Claims

1. A method for selecting lead-candidate compounds capable of binding to a biopolymer from a compound database containing three-dimensional structure information of compounds by using a computer, wherein one or more query compounds which are assumed to be capable of binding to a receptor biopolymer, or assumed to fit a virtual receptor model, or already known to be capable of binding to a receptor biopolymer are used as query molecules, structures of the compounds are modified to an extent that their binding to the biopolymer should not be retarded, and stability of complex structures of the biopolymer and the compounds is used as criteria for judgment.

2. A method for selecting lead-candidate compounds capable of binding to a biopolymer from a compound database containing three-dimensional structure information of compounds by using a computer, wherein one or more query compounds which are assumed to be capable of binding to a receptor biopolymer, or assumed to fit a virtual receptor model, or already known to be capable of binding to a receptor biopolymer are used as query molecules, structures of the compounds are modified to an extent that their binding to the biopolymer should not be retarded, stability of complex structures of the biopolymer and the compounds is used as criteria for judgment, and characterized by a first screening based on quantitative information including number of atoms and the like, a second screening based on information about atomic types and mode of covalent bonds, and a third screening based on structures of complexes formed with the biopolymer based on correspondence of atoms with those of the query molecules.

3. A method for selecting lead-candidate compounds capable of binding to a receptor biopolymer from a database containing, at least, information about atomic types and mode of covalent bonds of compounds by using a computer, which comprises the following step:
(a) a step of selecting lead-candidate compounds by matching one or more query molecules capable of binding to a biopolymer with compounds stored in a database based on information about atomic types and mode of covalent bonds of the query molecules.

4. The method of claim 3 wherein the database contains information about three-dimensional structure of the compounds.

5. The method of claim 3 or 4 which comprises a step (b) of constructing structures of the query compounds by an automatic structure construction method.

6. The method of any one of claims 3 to 5 wherein the step (a) comprises either or

both of the following two steps:

(c) a step of first screening by selection of trial compounds based on one or more parameters selected from a group of parameters consisting at least of number of atoms, number of bonds, number of ring structures, number of atoms for each atomic type and molecular weight; and/or

(d) a step of second screening by matching of candidate compounds selected in the first screening step for mode of covalent bonds.

7. The method of claim 6 wherein the step (d) comprises the following step:

(e) a step of second screening based on information about marker sites in the query molecules.

8. The method of any one of claims 3 to 7 wherein, after the step(a), a third screening is performed by the following step (f):

(f) a step of selecting one or more preferred lead-candidate compounds by estimating binding schemes to the biopolymer for the lead-candidate compounds selected in the step (a) based on three-dimensional information and binding schemes of the query molecules to the biopolymer, and calculating one or more parameters relating to interaction between the lead-candidate compounds and the biopolymer;

and/or the following step (g):

(g) a step of selecting one or more preferred lead-candidate compounds by supposing a virtual receptor model which represents physicochemical environment of the ligand binding site of the biopolymer based on information of three-dimensional structures of one or more known ligands capable of binding to the biopolymer, and then judging goodness of fit to the virtual receptor model for the lead-candidate compounds selected in the step (a).